4. SURFACE WATER AND SEDIMENT ALGORITHMS

The surface water compartment is assumed to be well-mixed and composed of two phases: pure water and suspended sediment material that contains the sorbed contaminants. Similarly, the sediment is modeled as a well-mixed compartment consisting of a phase sorbed to the benthic solids and a phase dissolved in the benthic pore water or interstitial water. The gas phase of the surface water compartment is considered to be negligible in terms of its impact on the movement of chemicals. The text box beginning on the next page provides a quick summary of the algorithms developed in this chapter and provides a definition of all parameters used.

4.1 CONCEPTUALIZATION OF THE SURFACE WATER AND SEDIMENT COMPARTMENTS

The behavior of chemicals in surface waters is determined by three factors: the rate of input, the rate of physical transport in the water system, and chemical reactivity. Physical transport processes are dependent to a large extent on the type of water body under consideration *i.e.*, oceans, seas, estuaries, lakes, rivers, or wetlands. Schnoor (1981) and Schnoor and MacAvoy (1981) have summarized important issues relating to surface-water transport. Fugacity models have been developed for lakes and rivers by Mackay et al. (1983a,1983b).

At low concentrations, contaminants in natural waters exist in both a dissolved and a sorbed phase. In slow-moving surface waters (*e.g.*, lakes), both advection and dispersion are important. In rapidly moving water systems (*e.g.*, rivers), advection controls mass transport, and dissolved substances move at essentially the same velocity as the bulk water in the system. A water balance is the first step in assessing surface-water transport. A water balance is established by equating gains and losses in a water system with storage. Water can be stored within estuaries, lakes, rivers, and wetlands by a change in elevation. Water gains include inflows (both runoff and stream input) and direct precipitation. Water losses include outflows and evaporation.

The accuracy of modeling fresh water systems depends on the ability to accurately simulate the movement of water and sediment to and from the system (Schnoor 1981). There are two primary categories for fresh water: rivers and lakes. This model is based on that described in Mackay et al. (1983a,1983b). Table 4-1 summarizes the gains and losses considered from the surface water compartment considered in the TRIM.FaTE prototype. Losses from the sediment due to colloidal diffusion, bioturbation, or reaction/transformation are not considered at this stage of the TRIM.FaTE model.

The general manner in which the model is presented is intended to assist the flexibility of future prototypes and to facilitate implementing different algorithms to describe specific processes. The use of the fugacity terminology is used to describe the advective process for simplicity of notation and consistency.

Summary of Transport Algorithms Developed in this Chapter

Dry deposition of particles to surface water (solid phase):

$$T^{dd}_{air \rightarrow sw} = \frac{A_{airsw}}{V_{air}} \upsilon_d \frac{\rho_a Z_{solid}}{\rho_p Z_{total}}$$

Wet deposition of particles to surface water (solid phase):

$$T^{wd}_{air \rightarrow sw} = \frac{A_{airsw}}{V_{air}} Wet_d \frac{\rho_a Z_{solid}}{\rho_p Z_{total}}$$

Advective flux from rainfall:

$$T_{i \rightarrow j}(rain) = A_{ij} \frac{Rain}{V_{air}} \frac{Z_{water}}{Z_{total}}$$

Deposition of suspended sediment to sediment bed (solid phase):

$$T^{d}_{sw \rightarrow sed} = \frac{A_{swsed}}{V_{sw}} \frac{S_{dep}}{\rho_{ss}} \frac{Z_{solid}}{Z_{total}}$$

Resuspension of sediment to surface water (solid phase):

$$T^{r}_{sed \rightarrow sw} = \frac{A_{sedsw}}{V_{sed}} \frac{S_r}{\rho_{bs}} \frac{Z_{solid}}{Z_{total}}$$

Outflow from surface water to surface water advection sink (total phase):

$$T_{sw \rightarrow s} = Outflow / V_{sw}$$

Resuspension of sediment to surface water (solid phase):

$$T^{total}_{sed \rightarrow sw} = \max\left(0, \frac{A_{sedsw}}{V_{sw}} \frac{S_{dep}}{\rho_{ss}} - \frac{A_{sed \rightarrow sw}}{V_{sed}} \frac{S_r}{\rho_{bs}}\right) \frac{Z_{solid}}{Z_{total}}$$

Advection from one river compartment to another river or lake compartment:

$$T^{adv}_{i \rightarrow j}(total) = \frac{A_{ij}}{V_i} u_{ij}$$

Dispersive exchange flux between two surface water compartments:

$$F_{i \rightarrow j} = \frac{E_{ij} \cdot A_{ij}}{L_{ij}} (C_j - C_i)$$

$$= \frac{E_{ij} \cdot A_{ij}}{L_{i \rightarrow j}} \left(\frac{M_j}{V_j} - \frac{M_i}{V_i} \right)$$

Summary of Transport Algorithms Developed in this Chapter (cont.)

where:

$T^{dd}_{air \rightarrow sw}$	=	advective transfer factor of particles from air to surface water (1/day)
$^{wd}_{air \rightarrow sw}$	=	advective transfer factor of wet particles from air to surface water (1/day)
$^{d}_{sw \rightarrow sed}$	=	advective transfer factor for deposition of suspended sediment to sediment bed (1/day)
$^{r}_{sed \rightarrow sw}$	=	advective transfer factor for resuspension of sediment to surface water (1/day)
$^{total}_{sed \rightarrow sw}$	=	net advective transfer factor for deposition and resuspension of sediment to surface water (1/day)
A_{airsw}	=	area of surface water/air interface (m^2)
V_{air}	=	volume of air compartment (m^3)
υ_d	=	dry deposition velocity of particles (m/day)
ρ_a	=	atmospheric dust load in air compartment (concentration of dust in air) (kg [particles]/m^3 [atmosphere])
ρ_p	=	density of air particles (kg [particles]/m^3 [particles])
Wet_d	=	wet deposition velocity of particles (m/day)
$Rain$	=	rainfall rate (m/day)
A_{swsed}	=	area of surface water/sediment interface (m^2)
V_{sw}	=	volume of surface water compartment (m^3)
S_{dep}	=	deposition rate of suspended sediment to sediment bed (kg [suspended sediment]/m^2 (area)-day)
ρ_{ss}	=	density of suspended sediment (kg [suspended sediment]/m^3 [suspended sediment])
A_{sedsw}	=	area of surface water/sediment interface (m^2)
V_{sed}	=	volume of sediment compartment (m^3)
S_r	=	resuspension rate of benthic sediment to water column (kg [benthic sediment]/m^2 (area)-day)
ρ_{bs}	=	density of benthic sediment (kg [benthic sediment]/m^3 [benthic sediment])
$Outflow$	=	outflow of water from surface water compartment to advection sink (m^3/day)
V_{sw}	=	volume of surface water compartment (m^3)
Z_{solid}	=	fugacity of the solid phase (Pa)
Z_{total}	=	total fugacity (Pa)
Z_{water}	=	fugacity of the water phase (Pa)
u_{ij}	=	averaged river flow between river compartments i and j (m/h)
C_i, C_j	=	concentration of chemical in water compartments *i* and *j* (g/m^3)
$F_{i \rightarrow j}$	=	dispersive flux from water compartment *i* to water compartment *j* (mass [chemical]/day)
M_i, M_j	=	mass of chemical in water compartments *i* and *j* mg/L (g)
E_{ij}	=	dispersion coefficient for exchange between water compartments *i* and *j* (m^2/day)
A_{ij}	=	interfacial area between water compartments *i* and *j* (m^2)
L_{ij}	=	characteristic mixing length between water compartments *i* and *j* (m)

Table 4-1
Summary of the Gains and Losses for Surface Water Compartments Considered in the Prototype

Gains	Type of Process	Relevant Phase	Losses	Type of Process	Relevant Phase
From Surface Soil					
Erosion	Advective	Solid			
Runoff	Advective	Aqueous			
From Air			**To Air**		
Diffusion from air	Diffusive	Vapor	Diffusion to air	Diffusive	Aqueous
Dry deposition of aerosols from air	Advective	Solid			
Wet deposition of aerosols from air	Advective	Solid			
Wet deposition of vapor from air	Advective	Vapor			
From Sediment			**To Sediment**		
Diffusion from sediment	Diffusive	Aqueous	Diffusion to sediment	Diffusive	Aqueous
Resuspension of sediment	Advective	Solid	Deposition to sediment	Advective	Solid
From Rivers			**To Lake**		
Compartment to compartment advective flow	Advective	Total	River to lake advective flow	Advective	Total
From Aquatic Biota			**To Aquatic Biota**		
Elimination from fish	Exchange	Total	Uptake by fish	Exchange	Total
From Surface Water Transformations			**To Sink(s)**		
			Decay/transformation to Reaction/Advection sink	Transformation	Total
			Outflow to Reaction/Advection sink	Advective	Total

4.2 ADVECTIVE PROCESSES

A generalized description of advective processes is provided in Section 2.3.1. This section focuses on the advective processes simulated in the prototype specific to the surface water compartment.

4.2.1 ADVECTIVE PROCESSES BETWEEN AIR AND SURFACE WATER

The advective processes considered between air and surface water are wet and dry deposition of solid phase particles and wet deposition of vapor that is dissolved into the water phase. For all of these processes, the air compartment is the sending compartment and the surface water compartment is the receiving compartment.

Following is a summary of advective processes between air and surface water, and algorithms used to calculate phase flow velocities:

Dry deposition of particles to surface water (solid phase):

$$T^{dd}_{air \rightarrow sw} = \frac{A_{airsw}}{V_{air}} \upsilon_d \frac{\rho_a Z_{solid}}{\rho_p Z_{total}} \tag{4-1}$$

where:

$T^{dd}_{air \rightarrow sw}$	=	advective transfer factor of particles from air to surface water (1/day)
A_{airsw}	=	area of surface water (m^2)
V_{air}	=	volume of air compartment (m^3)
υ_d	=	dry deposition velocity of particles (m/day)
ρ_a	=	atmospheric dust load in air compartment (concentration of dust in air) (kg [particles]/m^3 [atmosphere])
ρ_P	=	density of air particles (kg [particles]/m^3 [particles])
Z_{solid}	=	fugacity of the solid phase (Pa)
Z_{total}	=	total fugacity (Pa).

Wet deposition of particles to surface water (solid phase):

$$T^{wd}_{air \rightarrow sw} = \frac{A_{airsw}}{V_{air}} Wet_d \frac{\rho_a Z_{solid}}{\rho_p Z_{total}} \tag{4-2}$$

where:

$T^{wd}_{air \rightarrow sw}$	=	advective transfer factor of wet particles from air to surface water (1/day)
A_{airsw}	=	area of surface water/air interface (m^2)
V_{air}	=	volume of air compartment (m^3)
Wet_d	=	wet deposition velocity of particles (m/day)
ρ_a	=	atmospheric dust load in air compartment (concentration of dust in air) (kg [particles]/m^3 [atmosphere])
ρ_P	=	density of air particles (kg [particles]/m^3 [particles])
Z_{solid}	=	fugacity of the solid phase (Pa)
Z_{total}	=	total fugacity (Pa).

Additionally, there is advective flux from rainfall. As the rain falls, it gathers chemical from the air, coming into equilibrium with the fugacity of the air compartment.

Advective flux from rainfall:

$$flux(g/day) = A_{ij}\ \frac{Rain}{V_i}\ \frac{Z_{water}}{Z_{Total}}\ N_a$$
$$\Rightarrow \qquad T_{i\to j}(rain) = A_{ij}\ \frac{Rain}{V_i}\ \frac{Z_{water}}{Z_{Total}} \tag{4-3}$$

where:

$Rain$	=	rainfall rate (m/day)
N_a	=	total mass of chemical in the air compartment (g)
Z_{water}	=	fugacity of the water phase (Pa)
Z_{total}	=	total fugacity (Pa).

4.2.2 ADVECTIVE PROCESSES BETWEEN SEDIMENT AND SURFACE WATER

The two advective processes between sediment and surface water involve the transport of the chemical from the surface water to the sediment or from the sediment to the surface water via movement of sediment particles. “Sediment deposition” refers to the transport of the chemical from the surface water to sediment, and “sediment resuspension” refers to the reverse process. Both processes involve only the solid phase.

Following is a summary of advective processes between sediment and surface water, and algorithms used to calculate phase flow velocities:

Deposition of suspended sediment to sediment bed (solid phase):

$$T^{d}_{sw\rightarrow sed} = \frac{A_{swsed}}{V_{sw}} \frac{S_{dep}}{\rho_{ss}} \frac{Z_{solid}}{Z_{total}} \tag{4-4}$$

where:

$T^{d}_{sw\rightarrow sed}$	=	advective transfer factor for deposition of suspended sediment to sediment bed (1/day)
A_{swsed}	=	area of surface water/sediment interface (m^2)
V_{sw}	=	volume of surface water compartment (m^3)
S_{dep}	=	deposition rate of suspended sediment to sediment bed (kg [suspended sediment]/m^2 (area)-day)
ρ_{ss}	=	density of suspended sediment (kg [suspended sediment]/m^3 [suspended sediment])
Z_{solid}	=	fugacity of the solid phase (Pa)
Z_{total}	=	total fugacity (Pa).

Resuspension of sediment to surface water (solid phase):

$$T^{r}_{sed \rightarrow sw} = \frac{A_{sedsw}}{V_{sed}} \frac{S_r}{\rho_{bs}} \frac{Z_{olid}}{Z_{total}} \tag{4-5}$$

where:

$T^{r}_{sed \rightarrow sw}$	=	advective transfer factor for resuspension of sediment to surface water (1/day)
A_{sedsw}	=	area of surface water/sediment interface (m^2)
V_{sed}	=	volume of sediment compartment (m^3)
S_r	=	resuspension rate of benthic sediment to water column (kg [benthic sediment]/m^2 (area)-day)
ρ_{bs}	=	density of benthic sediment (kg [benthic sediment]/m^3 [benthic sediment])
Z_{solid}	=	fugacity of the solid phase (Pa)
Z_{total}	=	total fugacity (Pa).

4.2.3 ADVECTIVE PROCESSES BETWEEN SEDIMENT/SURFACE WATER AND ADVECTIVE SINKS

The surface water advection sink represents outflow of the chemical from the study area. For sediment, the advection sink represents the burial of the chemical beneath the sediment layer.

Burial is calculated so that the net flow of sediment into the sediment layer is zero. That is, there is no loss of sediment mass due to burial, only loss of pollutant. This is done by setting the amount of sediment buried equal to the sediment deposition rate minus the sediment resuspension rate, both of which are specified input parameters. If the resuspension rate is larger than the deposition rate, then the burial flow is set to 0. A more sophisticated approach may be implemented in which the sediment layer depth could change, depending on the deposition and resuspension rates. Further, the deposition rates can be calculated to correspond to the suspended sediment concentration, which could change depending on the erosion of soil to the water body and the outflow.

Following is a summary of advective processes between sediment/surface water and advective sinks, and algorithms used to calculate flow velocities:

Outflow from surface water to surface water advection sink (total phase):

$$T_{sw \rightarrow s} = Outflow / V_{sw} \tag{4-6}$$

where:

Outflow	=	outflow of water from surface water compartment to advection sink (m^3/day)
V_{sw}	=	volume of surface water compartment (m^3)

Resuspension of sediment to surface water (solid phase):

$$T_{sedsw}^{total} = \max\left(0, \frac{A_{sedsw}}{V_{sw}}\frac{S_{dep}}{\rho_{ss}} - \frac{A_{sed\rightarrow sw}}{V_{sed}}\frac{S_r}{\rho_{bs}}\right)\frac{Z_{solid}}{Z_{total}} \qquad (4\text{-}7)$$

where:

T_{sedsw}^{total}	=	net advective transfer factor for deposition and resuspension of sediment to surface water (1/day)
A_{sedsw}	=	area of surface water/sediment interface (m^2)
V_{sed}	=	volume of sediment compartment (m^3)
S_r	=	resuspension rate of benthic sediment to water column (kg [benthic sediment]/m^2 (area)-day)
ρ_{bs}	=	density of benthic sediment (kg [benthic sediment]/m^3 (benthic sediment])
V_{sw}	=	volume of surface water compartment (m^3)
S_{dep}	=	deposition rate of suspended sediment to sediment bed (kg [suspended sediment]/m^2 (area)-day) (Mackay et al. 1983b; use 0.096 m^3/hr for a lake of volume 7 x 10^{-6} m)
ρ_{ss}	=	density of suspended sediment (kg [suspended sediment]/m^3 [suspended sediment])
Z_{solid}	=	fugacity of the solid phase (Pa)
Z_{total}	=	total fugacity (Pa).

4.3 DERIVATION OF RIVER COMPARTMENT TRANSFER FACTORS

The transfer factor from one river compartment to another, or to a lake compartment, was derived based on advective flow rates of a total pollutant mass between two compartments as developed in Section 2.3.1. By substituting river flow velocity for the total volumetric flow velocity, the following transfer factor is derived.

Advection from one river compartment to another river or lake compartment:

$$T_{ij}^{adv}(total) = \frac{A_{ij}}{V_i} u_{ij} \qquad (4\text{-}9)$$

where:

u_{ij} = annual averaged river flow between river compartments i and j (m/day)
A_{ij} = area of interface between compartments i and j (m^2)
V_i = volume of compartment i (m^3).

Because advection is being simulated for the total phase, no phase partitioning is applied in this equation.

4.4 DISPERSIVE PROCESSES

4.4.1 DISPERSIVE TRANSPORT BETWEEN SURFACE WATER COMPARTMENTS

Dispersive transport between water compartments can be approximated as a first order process using the method describe in the WASP water quality simulation program (Ambrose et al.1995). Dispersive water column exchanges significantly influence the transport of dissolved and particulate pollutants in such water bodies as lakes, reservoirs, and estuaries. Even in rivers, longitudinal dispersion can be the most important process diluting peak concentrations that may result from unsteady loads or spills.

Based on the WASP model, the dispersive exchange flux between two surface water compartments i and j at time is modeled by:

$$\begin{aligned} F_{i \to j} &= \frac{E_{ij} \cdot A_{ij}}{L_{ij}} (C_j - C_i) \\ &= \frac{E_{ij} \cdot A_{ij}}{L_{ij}} \left(\frac{M_j}{V_j} - \frac{M_i}{V_i} \right) \end{aligned} \tag{4-10}$$

where:

$F_{i \to j}$ = dispersive flux from water compartment i to water compartment j (mass [chemical]/day)
C_i, C_j = concentration of chemical in water compartments i and j (g/m^3)
M_i, M_j = mass of chemical in water compartments i and j (g/m^3)
E_{ij} = dispersion coefficient for exchange between water compartments i and j (m^2/day)
A_{ij} = interfacial area between water compartments i and j (m^2)
L_{ij} = characteristic mixing length between water compartments i and j (m)
V_i = volume of compartment i (m^3)
V_j = volume of compartment j (m^3).

The distance between the midpoints of the two water compartments is used for the characteristic mixing length. Values for dispersion coefficients can range from 10^{-10} m^2/sec (8.64x

10^{-6} m^2/day) for molecular diffusion to $5x10^2$ m^2/sec ($4.32x10^7$ m^2/day)for longitudinal mixing in estuaries (Ambrose et al. 1995, p. 35). A value of $2.25x10^{-4}$ m^2/day is chosen as the default value; this is median of the range cited in Ambrose et al. (1995) (p. 112) from a study of Lake Erie conducted by Di Toro and Connolly (1980).

4.4.2 DISPERSIVE TRANSPORT BETWEEN SURFACE WATER AND SEDIMENT COMPARTMENTS

As for dispersive transport between surface water compartments, dispersive transport between surface water and sediment compartments is approximated as a first order process using the method described in the WASP water quality simulation program (Ambrose et al. 1995).

Based on the WASP model, the net dispersive exchange flux between a surface water compartment *i* and sediment compartment *j* is modeled by:

$$\begin{aligned} F_{j \to i} &= \frac{E_{ij} \cdot A_{ij}\, n_{ij}}{L_{ij}/n_{ij}} \left(\frac{f_{Dj}\, C_j}{n_j} - \frac{f_{Di}\, C_i}{n_i} \right) \\ &= \frac{E_{ij} \cdot A_{ij}\, n_{ij}}{L_{ij}/n_{ij}} \left(\frac{f_{Dj}\, M_j}{V_j n_j} - \frac{f_{Di}\, M_i}{V_i n_i} \right) \end{aligned} \qquad (4\text{-}11)$$

where:

$F_{j->i}$	=	Net dispersive flux between surface water compartment *i* and sediment compartment *j*, mass[chemical]/day
C_i, C_j	=	Bulk concentration of chemical in surface water compartment *i* and sediment compartment *j* mg/L (g[chemical]/m^3[compartment])
M_i, M_j	=	Mass of chemical in surface water compartment *i* and sediment compartment *j* (mass[chemical])
E_{ij}	=	Dispersion coefficient for exchange between compartments *i* and *j*, m^2/day
A_{ij}	=	Interfacial area between compartments *i* and *j*, m^2
L_{ij}	=	Characteristic mixing length between compartments *i* and *j*, m
V_i , V_j	=	volume of compartments *i* and *j*, m^3
f_{Di}, f_{Dj}	=	dissolved fraction of chemical in compartments *i* and *j* (calculated)
n_i, n_j	=	porosity of compartments *i* and *j*
n_{ij}	=	average porosity at interface ($(n_i + n_j)/2$)

The resulting transfer factors (units of */day*) between the surface water *i* and sediment compartment *j* are given by:

$$T_{i \to j} = \frac{E_{ij} \cdot A_{ij}\, n_{ij}}{L_{ij}/n_{ij}} \left(\frac{f_{Di}}{V_i n_i} \right) \tag{4-12}$$

$$T_{j \to i} = \frac{E_{ij} \cdot A_{ij}\, n_{ij}}{L_{ij}/n_{ij}} \left(\frac{f_{Dj}}{V_j n_j} \right) \tag{4-13}$$

Following the method used in WASP (Amborse et al., p. 25), the sediment compartment height is used as the characteristic mixing length L_{ij}. The porosity of the sediment compartment (n_j) is calculated from the specified benthic solids concentration and solids density. The porosity of the surface water compartment is set to the volume of water compartment that is water. Values for dispersion coefficients can range from 10^{-10} m^2/sec ($8.64x10^{-6}$ m^2/day) for molecular diffusion to $5x10^2$ m^2/sec ($4.32x10^7$ m^2/day)for longitudinal mixing in estuaries (Ambrose et al. 1995, p. 35). A value of 2.25e-4 m^2/day is chosen as the default value; this is median of the range cited in Ambrose et al. 1995 [p. 112] from a study of Lake Erie conducted by DiToro and Connolly (1980).

4.5 DIFFUSIVE PROCESSES

4.5.1 DIFFUSIVE EXCHANGE BETWEEN SURFACE WATER AND AIR

The algorithms describing the diffusive exchange of chemical mass between surface water and air are presented in Section 3.3.2.

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